

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Transport of nanoparticles in porous media with Dissipative Particle Dynamics (DPD) simulation¹ MINH VO, DIMITRIOS PAPAVALASSILIOU, The University of Oklahoma — Nanoparticles can serve as nanosensor devices in oil recovery processes, because of their ability to propagate in porous media. We employ DPD simulations to explore the factors affecting the retention and mobility of carbon nanotubes (CNT) in porous media. Compared to molecular dynamics simulations, longer time and length scales can be obtained with DPD, while the hydrodynamic properties of system are also maintained. Besides, complex flow structures can be handled by DPD in a simple manner (using frozen DPD beads for solid surface). In our calculations, packed-sphere geometry is utilized to create porous media. After equilibrium, CNTs are released into the flow. The interaction between the CNTs and the solid surface is considered by applying both shifted force Lenard-Jones and Morse potential in the DPD model. Different sizes of CNTs are investigated, in order to study the effect of the aspect ratio on the hydrodynamic forces as well as the rotation of CNTs while moving with the flow. In addition, the mobility of CNTs is discussed by computing their trajectory in the flow and comparing the cylindrical particles to spherical.

¹This work was supported by the Advanced Energy Consortium. The use of computing facilities at OSCER and at XSEDE (CTS-090025) is also acknowledged

Dimitrios Papavassiliou
The University of Oklahoma

Date submitted: 14 Nov 2013

Electronic form version 1.4